Accelerating materials discovery using artificial intelligence, high performance computing and robotics

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Abstract

New tools enable new ways of working, and materials science is no exception. In materials discovery, traditional manual, serial, and human-intensive work is being augmented by automated, parallel, and iterative processes driven by Artificial Intelligence (AI), simulation and experimental automation. In this perspective, we describe how these new capabilities enable the acceleration and enrichment of each stage of the discovery cycle. We show, using the example of the development of a novel chemically amplified photoresist, how these technologies' impacts are amplified when they are used in concert with each other as powerful, heterogeneous workflows.